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13. ABSTRACT (Maximum 200 words)

A number of improvements to PDEPACK have been made. These include the development of parallel discretization methodologies and sparse/iterative PDE solvers.



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# FINAL REPORT FOR AFOSR CONTRACT F49620-92-J-0069 High Performance Computing Methods and Systems for Partial Differential Equations

Period September 1, 1992 - February 28, 1995

July 19, 1995

### A. PROJECT RESULTS

In this report we list the personnel that worked under this AFOSR grant, the publications completed and describe the accomplishments of various projects. The results under this contract include:

PDEPACK: The PDE solving system PDEPACK has been designed and a prototype made operational. Its objectives are

- Provide a software framework for PDE solving,
- Integrate major public domain PDE solvers and libraries,
- develop parallel discretization methodologies and sparse/iterative solvers.

The status of the software in PDEPACK is as follows:

## Already Incorporated

ELLPACK MGGAT //ELLPACK PATRAN FIDISOL **PCGPACK** VECTEM PDECOL NSPCG PDEONE LINPACK Sparskit CVD RCTR VERSE CADSOL CFD

In Process of Being Incorporated

PTS

PDETWO

OCEAN

MP PCGPACK2

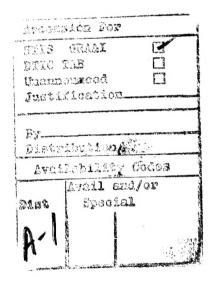
Being Studied for Incorporation

LAPACK

ACM Algorithms 392,494,533,572,593,651

**IMSL** 

DLEARN



PDELab: PDEPACK is the basis for PDELab, a problem solving environment for high performance PDE applications. Its objectives are

- · A generic environment to specify PDE models,
- A unified interactive PDE solving environment,
- Assistance in making decisions at all levels of PDE solving.

The software architecture for PDELab has been completed and a prototype is operational. PDE-Lab is a general problem solving environment for high performance PDE based applications; it is based on the solvers in PDEPACK. Two application specific problem solving environments have been designed to be built on top on PDELab. One, called BioSeparation Lab, is operational. It incorporates a PDE model of the chemical engineering process along with online connections to actual experimental apparatus so the process can be controlled. The second one is still being built; it is to model and control the Chemical Vapor Deposition process used to make microchip wafers.

PYTHIA: The PDELab prototype incorporates the expert system PYTHIA which

- Uses exemplar and neuro-fuzzy based learning to guide the selection of software and hardware for PDE applications.
- Has a knowledge base facility that automatically generates value to support "smart" sequential and parallel PDE solvers.

WWW Servers: A prototype World Wide Web based server for PDELab has been designed and is operational. It allows a user on the internet to solve elliptic PDEs using //ELLPACK (a subset of PDELab) on our server and its associated parallel machines. This systems is being enhanced and extended for all of PDELab.

Basic Research: A variety of more basic research results have been obtained to:

- (a) Analyze the performance of parallel computation
- (b) Analyze numerical methods for partial differential equations
- (c) Analyze the partitioning of PDE problems for parallel computation.

# B. PERSONNEL

Work on this grant has involved the following people:

John R. Rice\*(Co-PI) Professor of Computer Science
Elias N. Houstis\*(Co-PI) Professor of Computer Science

Apostolos Hadjidimos\* Visiting Professor of Computer Science

Catherine E. Houstis Visiting Assoc. Professor of Computer Science

Cheryl Crabill\* Programmer
Manolis Vavalis\* Postdoc
Mo Mu\* Postdoc
Ko Yang Wang\* Postdoc

Nicholas Chrisochoides\* Ph.D. candidate Sanjiva Weerawarana\* Ph.D. candidate Sang Bae Kim Ph.D. candidate Scott McFadden Ph.D. candidate Hveran Bvun Ph.D. candidate Yu-Ling Lai Ph.D. candidate Po-Ting Wu Ph.D. candidate Mei-Ling Shvu\* Ph.D. candidate Chi Chui\* Ph.D. candidate Winnie Lap-kan Ng\* Ph.D. candidate Pelayia Varodoglu M.S. student Jim Berniger\* M.S. student Athanasios Gaitatzes M.S. student

Margaret Gaitatzes M.S. student, Programmer

Shahani Weerawarana M.S. student Hongtao Gu\* M.S. student Konstantios Pantazopoulos\* M.S. student Jeffrey Michael\* M.S. student

Meletis Samartzis\* Visiting Research Associate

Stavros Kortesis Visiting Scholar

Those names with stars have received some direct AFOSR support, the others have research support from related projects.

### C. EXTERNAL HONORS

John R. Rice :

- ACM Service Award: Assoc. Comp. Mach., March 1993.
- CRA Service and Leadership Award: Computing Research Assoc., July 1993.
- Elected to National Academy of Engineering, 1994.
- Sigma Xi Award for Outstanding Research by Purdue Faculty Member, 1994.
- Appointed to editorial board of IEEE Computational Science and Engineering, 1994.

• Appointed Academic Advisory Board of Industrial Research Institute, 1995.

# D. PUBLICATIONS

We list the publications that have resulted from the past three years of work supported by the AFOSR. These include:

- 13 Journal papers
- 3 Papers submitted for journal publication
- 14 Refereed Conference papers
- 1 Book edited
- 1 Ph.D. Thesis
- 7 Papers in books/proceedings

# 1. REFEREED JOURNALS

- 1. H.S. McFadden and J.R. Rice, Collaborating PDE solvers. Applied Numerical Mathematics, 10, (1992), 279–295.
- 2. M. Mu and J.R. Rice, Row oriented Gauss elimination on distributed memory multiprocessors. *Intl. J. High Speed Comp.*, 4, (1992), 143-168.
- 3. A. Hadjidimos, E.N. Houstis, E.A. Vavalis, and J.R. Rice, Iterative line cubic spline collocation methods for elliptic partial differential equations in several dimensions. SIAM J. Sci. Stat. Comp., 14 (1993), 715-734.
- 4. M. Mu and J.R. Rice, An organization of sparse Gauss elimination for solving partial differential equations on distributed memory machines. *Numer. Meth. Part. Diff. Eqns.*, 9 (1993), 175–189.
- 5. D.C. Marinescu and J.R. Rice, On high level characterization of parallelism. J. Par. Dist. Comp., 20 (1994), 107-113.
- 6. M. Mu and J.R. Rice, Preconditioning for domain decomposition through functional approximation. SIAM J. Sci. Comp., 15 (1994), 1452-1466.
- 7. N. Chrisochoides, E.N. Houstis, and J.R. Rice, Mapping algorithms and software environments for data parallel PDE iterative solvers. J. Par. Dist. Comp., 21, (1994), 75-95.
- 8. Y.-L. Lai, A. Hadjidimos, E.N. Houstis, and J.R. Rice, General interior hermite collocation methods for second order elliptic partial differential equations. *Applied Numerical Methods*, (1995), to appear.

- D.C. Marinescu, J.R. Rice, and E.A. Vavalis, Performance of iterative methods for distributed memory machines. Applied Numerical Mathematics, 12 (1994), pp. 421-430. Extended abstract in Proc. 13th World Congress, IMACS, Rutgers University, New Brunswick, NJ, Vol. 2 (1991), 684-685.
- 10. D.C. Marinescu and J.R. Rice, On the scalability of asynchronous parallel computations. J. Par. Dist. Comp., 22 (1994), 538-546.
- 11. E. Gallopoulos, E.N. Houstis, and J.R. Rice, Computer as thinker/doer: Problem solving environments for computational science. *IEEE Comp. Sci. Engr.*, 1 (1994), 11-23.
- 12. J. Lambers and J.R. Rice, QUAD2D: Adaptive quadrature for general two dimensional domains, submitted as paper and companion algorithm.
- 13. S.B. Kim, A. Hadjidimos, E.N. Houstis, and J.R. Rice, Multi-parameterized Schwarz splittings, submitted to *Numerical Linear Algebra and Applications*.
- 14. A. Hadjidimos and D. Noutsos, On a matrix identity connecting iteration operations associated with a p-cyclic matrix, *Linear Algebra Appl.*, **182** (1993), 157-177.
- 15. A. Hadjidimos and M. Neumann, On domains of superior convergence of the SSOR method over the SOR method, *Linear Algebra Appl.*, **187** (1993), 67-85.
- 16. M. Mu and J.R. Rice, Modeling with collaborating PDE solvers Theory and practice. Contemporary Mathematics, 180, (1994), 427-438.

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- 17. A. Hadjidimos and R.J. Plemmons, Analysis of p-cyclic iterations for Markov chains, in *Linear Algebra, Markov Chains, and Queueing Models*, (C.D. Meyer and R.J. Plemmons, eds.), IMA Series on Applied Mathematics, Springer-Verlag, 48 (1993), 111-124.
- 18. M. Mu and J.R. Rice, A PDE sparse solver benchmark for massively parallel distributed memory multiprocessors. In *Computer Methods for Partial Differential Equations VII* (R. Vichnevetsky, ed.), IMACS, New Brunswick, NJ (1992), 546-552.
- E.N. Houstis and J.R. Rice, The architecture of PDE solving systems. In Computer Methods for Partial Differential Equations VII (R. Vichnevetsky, ed.), IMACS, New Brunswick, NJ (1992), 363-370.
- N. Chrisochoides, E.N. Houstis, S.B. Kim, M.K. Samartzis, and J.R. Rice, Parallel iterative methods. In Computer Methods for Partial Differential Equations VII (R. Vichnevetsky, ed.), IMACS, New Brunswick, NJ (1992), 134-141.

- 21. N. Chrisochoides and J.R. Rice, Partitioning heuristics for PDE computations based on parallel hardware and geometry characteristics. In *Computer Methods for Partial Differential Equations VII* (R. Vichnevetsky, ed.), IMACS, New Brunswick, NJ (1992), 127-133.
- 22. C. E. Houstis, E.N. Houstis, J.R. Rice, S.M. Weerawarana, and S. Weerawarana, PYTHIA: An expert system for the support of smart parallel PDE solvers, *Third International Conference on Expert Systems for Numeric Computing* (E.N. Houstis and J. R. Rice, eds.), May 1993.
- 23. E.N. Houstis, J.R. Rice, S.M. Weerawarana, and S. Weerawarana, ParPDElab: A problem solving environment for the development of PDE based applications on parallel machines. *Third International Conference on Expert Systems for Numeric Computing* (E.N. Houstis and J.R. Rice, eds.), May 1993.
- 24. D.C. Marinescu and J.R. Rice, Speedup, communication complexity and blocking a la recherche du temps perdue. *Proc. 7th Intl. Par. Proc. Symp.*, IEEE Press, Los Alamitos, CA (1993), 712-721.
- 25. A. Catlin, C. Chui, C. Crabill, E.N. Houstis, S. Markus, J.R. Rice, and S. Weerawarana, PDELab: An object-oriented framework for building problem solving environments for PDE based applications, submitted to a conference.
- P. Wu, E.N. Houstis, and J.R. Rice, EPPOD: A parallel problem solving environment for the electronic prototyping of physical objects design, Proc. DAGS '94 Symposium, (F. Makedon, ed.), Dartmouth Inst. Adv. Grad. Studies. Dartmouth, NH (1994), 135-151.
- 27. E.N. Houstis. S. Weerawarana, A. Joshi, and J.R. Rice, The PYTHIA project, First Intl. Conf. on Neural, Parallel and Scientific Computations, 1995.
- 28. A. Joshi, S. Weerawarana, and E.N. Houstis, Using neural networks to support intelligent scientific computing, *Proceedings IEEE Intl. Conf. Neural Networks*, Orlando, 1995.
- 29. A. Joshi, T. Drashansky, E.N. Houstis, S. Weerawarana, SciencePad: An intelligent electronic notepad for ubiquitous scientific computing, IASTED/ISMM International Conference on Intelligent Information Management Systems, June 1995, Washington, D.C.
- 30. P. Wu and E.N. Houstis, A parallel mesh generation and decomposition methodology, *Proceedings of Mesh Generation Conference*, Albuquerque, October 1994.

# 3. BOOKS. BOOK CHAPTERS, AND PUBLICATIONS IN BOOKS/PROCEEDINGS

# 3.A. Books

- 31. E.N. Houstis and J.R. Rice, Artificial Intelligence, Expert Systems and Symbolic Computing, North-Holland, Amsterdam (1992).
- 32. S. Weerawarana, Problem Solving Environments for Partial Differential Equation Based Systems, Ph.D. Thesis, Department of Computer Sciences, Purdue University, 1994.

# 3.B. Publications in Books and Proceedings

- 33. P. Wu, E.N. Houstis, and J.R. Rice, Geometry as a basis for parallel analysis and design of physical objects, *Second U.S. National Congress on Computational Mechanics* (A.N. Noor, ed.), 1993.
- 34. R. Sharma and J.R. Rice, Numerical technique to solve nonlinear elliptic PDE's arising from semiconductor device modeling, *Proc. Intl. Workshop on Computational Electronics*, Beckman Inst., Univ. Illinois (1992), 123–126.
- 35. M. Mu and J.R. Rice, Preconditioner construction with rational approximation. In *Parallel Processing for Scientific Computing, II* (Sinovec, et. al., eds), SIAM Pub., Philadelphia (1993), 678-682.
- 36. E.N. Houstis, J.R. Rice, and S. Weerawarana, An open structure of PDE solving systems, *Proc. 14th IMACS World Congress*, IMACS **3** (1994), 1296–1299.
- 37. M.A. Corena-Hasegan, C. Costian, D.C. Marinescu, I. Martin, and J.R. Rice, Towards problem solving environments for high performance computing, *High Performance Computing Conference* '94, Nat. Supercomputer Res. Ctr., Singapore (1994), 354-366.
- 38. A. Hadjidimos, Y.-L. Lai and E.N. Houstis, A generalized Schwartz splitting method based on Hermite collocation for elliptic boundary value problems, CSD-TR-93-074, Computer Sciences Department, Purdue University, West Lafayette, IN, December 1993, Submitted.
- 39. E.N. Houstis, J.R. Rice, and S. Weerawarana, A software platform for integrating symbolic computation with a PDE solving environment. *Proc. 14th IMACS World Congress*, IMACS 1, (1994), 482–485.